

Attainable entanglement of unitary transformed thermal states in liquid-state nuclear magnetic resonance with the chemical shift

Yukihiro Ota,^{1,*} Shuji Mikami,¹ Motoyuki Yoshida,^{1,†} and Ichiro Ohba^{1,2,3,‡}

¹*Department of Physics, Waseda University, Tokyo 169-8555, Japan*

²*Kagami Memorial Laboratory for Material Science and Technology, Waseda University, Tokyo 169-0051, Japan*

³*Advanced Research Center for Science and Technology, Waseda University, Tokyo 169-8555, Japan*

(Dated: December 21, 2006)

Recently, Yu, Brown, and Chuang [Phys. Rev. A **71**, 032341 (2005)] investigated the entanglement attainable from unitary transformed thermal states in liquid-state nuclear magnetic resonance (NMR). Their research gave an insight into the role of the entanglement in a liquid-state NMR quantum computer. Moreover, they attempted to reveal the role of mixed-state entanglement in quantum computing. However, they assumed that the Zeeman energy of each nuclear spin which corresponds to a qubit takes a common value for all; there is no chemical shift. In this paper, we research a model with the chemical shifts and analytically derive the physical parameter region where unitary transformed thermal states are entangled, by the positive partial transposition (PPT) criterion with respect to any bipartition. We examine the effect of the chemical shifts on the boundary between the separability and the nonseparability, and find it is negligible.

PACS numbers: 03.67.Mn, 03.67.Lx

I. INTRODUCTION

Quantum mechanics has very different conceptual and mathematical characters from classical mechanics. The superposition and the entanglement (nonseparability) of quantum states make the difference clear. Recently, these characterizations have been utilized for a newly developing quantum technology. Actually, quantum entanglement is deeply related to quantum information processing (QIP) [1].

The role of entanglement in quantum computing has been researched from various viewpoints. In particular, the generation of entangled states by quantum dynamics, or quantum algorithms, will give us useful information on the above task [2, 3]. Recently, Yu, Brown, and Chuang [3] investigated the entanglement of unitary transformed thermal states in a liquid-state nuclear magnetic resonance (NMR) quantum computer. Such states are defined as the density matrices transformed from the thermal state in it by a specific class of unitary operators. We call the unitary transformations Bell-transformations. Their definition will be explained in Sec. II B. Furthermore, we call such states Bell-transformed thermal states. The thermal state in Ref. [3] is separable (i.e., there is no quantum correlation) [4] and characterized by two physical parameters: The one is the number of qubits, and the other is a measure of the state's polarization. The authors in Ref. [3] studied two kinds of Bell-transformations. One of their central interests is the difference between the Bell-transformed thermal states and effective pure states. The effective pure state

is the convex sum of the identity operator and a pure state, and a typical one is used in the current liquid-state NMR quantum computer [5, 6, 7]. They concluded that the former should be more easily entangled than the latter; the Bell-transformed thermal states can be entangled even in the physical parameter region where effective pure states are separable.

Their research is very important for the following three reasons. First, it gives an insight into the role of the entanglement in a liquid-state NMR quantum computer. Braunstein *et al.* [8] pointed out that the effective pure states should be almost separable in the current liquid-state NMR experiments. After their study, various studies on the role of entanglement in liquid-state NMR quantum computing were done (see Ref. [3] for additional references). One should note that the most natural quantum state is the thermal one in the liquid-state NMR and an effective pure state is constructed from it by a sequential operation of several quantum gates. Therefore, the authors in Ref. [3] investigated the entanglement of a more elementary state than effective pure states in liquid-state NMR quantum computers. Secondly, they attempted to reveal the role of mixed-state entanglement in quantum computing. Its evaluation and the meaning of mixed states will be more subtle than the case of pure states. Nevertheless, they can be characterized from the viewpoint of quantum communication. In particular, distillability is important [9, 10, 11]. If a mixed state is distillable, it is useful for QIP (e.g., quantum teleportation); we can distill a maximal entangled state by using a number of the copies, and local operations and classical communication (LOCC). Accordingly, their research could lead to the alternative understanding of mixed-state entanglement from the viewpoint of quantum computing. Finally, as mentioned in the beginning of this section, their work is related to the generation of entanglement by quantum dynamics. Actually, they

*Electronic address: oota@hep.phys.waseda.ac.jp

†Electronic address: motoyuki@hep.phys.waseda.ac.jp

‡Electronic address: ohba@waseda.jp

found the difference of the entanglement generation between the two Bell-transformations.

In this paper, we analytically derive the physical parameter region where the Bell-transformed thermal states are entangled in a more general case; specifically, the effect of the chemical shift [7, 12] is included in our Hamiltonian. The authors in Ref. [3] assumed that the Zeeman energy of each nuclear spin which corresponds to a qubit is a common value for all. However, it implies that one can't access the individual qubit; it is not a realistic model. Including such an effect is interesting from the theoretical point as well. When there is no chemical shift, the thermal state is a high symmetric one; the density matrix for such a state and the z component of the total spin operator commute. In our model, such a symmetry no longer exists. Therefore, our research may clarify a connection between the generation of entanglement by quantum gates and the symmetry of the system. Our method of evaluating the entanglement is simple and straightforward: Positive partial transposition (PPT) criterion [13, 14]. We analytically calculate the eigenvalues of the partial transposed Bell-transformed thermal states and find the least ones. Here, we would like to emphasize that, in Ref. [3], the Dür-Cirac classification [15] has been applied to the evaluation of the entanglement about two types of Bell-transformed thermal states, but it doesn't necessarily work in all cases.

This paper is organized as follows. In Sec. II, we introduce the Hamiltonian and the Bell-transformations. As in Ref. [3], we concentrate on two unitary operators of Bell-transformations. In Sec. III, in the first, we explain how to specify an individual bipartition and briefly review the PPT criterion. Next, we explain the Bell-diagonal state [16], which plays a central role in this paper. Then, we show the main results in Sec. III D: The sufficient conditions for the nonseparability of the Bell-transformed thermal states with respect to any bipartition. In Sec. IV, we show the necessary conditions for the full separability and the full distillability. In particular, we show the necessary and sufficient conditions for their full distillability when there is no chemical shift. In Sec. V, we examine the effect of the chemical shift on the boundary between the separability and the nonseparability determined by the PPT criterion. We summarize our results in Sec. VI. Furthermore, we briefly review the Dür-Cirac classification and show some examples which this method doesn't work in Appendix. A.

II. MODEL

A. Hamiltonian

In a liquid-state NMR quantum computer, the qubit is the nuclear spin in the molecule. We assume the number of the qubits is N in one molecule. The dipole-dipole interaction between the molecules in solutions are negligible because they randomly collide with each

other [7]. Therefore, we concentrate on the internal degrees of freedom (i.e., the nuclear spin) of one molecule. Let us define the computational bases as $|0\rangle_i$ and $|1\rangle_i$ (${}_i\langle 0|0\rangle_i = 1$, ${}_i\langle 1|1\rangle_i = 1$, and ${}_i\langle 0|1\rangle_i = 0$). The subscription $i(= 1, 2 \dots N)$ is the label of the qubit. Furthermore, we introduce the following standard operators: $I_i = |0\rangle_i\langle 0| + |1\rangle_i\langle 1|$, $Z_i = |0\rangle_i\langle 0| - |1\rangle_i\langle 1|$, $X_i = |0\rangle_i\langle 1| + |1\rangle_i\langle 0|$, and $H_i = (Z_i + X_i)/\sqrt{2}$. We analyze the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \frac{h\nu_i}{2} Z_i, \quad (1)$$

where $h\nu_i$ is the Zeeman energy of the i th qubit. Note that we neglect the J -coupling between the neighboring qubits because it is much smaller than the Zeeman energy in a liquid-state NMR [7, 12]. In this paper, we don't mention the relationship between the above computational basis and the physical spin state, and the Hamiltonian (1) is a mathematical model. We assume $h\nu_i$ is positive when we derive our main results. However, the model includes the important physical effect; every value of $h\nu_i$ is different from each other, due to the chemical shift. The effect allows us to access each qubit individually. In Ref. [3], every $h\nu_i$ is a common value. In this case, the Hamiltonian (1) and the z component of the total spin operator $J_z = \sum_{i=1}^N Z_i/2$ commute: $[\mathcal{H}, J_z] = 0$.

B. Bell-transformed thermal states

Let us consider the separable state which is characterized by a set of physical parameters. Our interest is the parameter region in which the state transformed from a separable one by quantum gates is a nonseparable one. Therefore, we have to specify a suitable initial separable state and quantum gates which generate the entanglement in a liquid-state NMR quantum computer.

First, we refer to the initial separable state. The system in a liquid-state NMR experiment is a thermal equilibrium state with high temperature. Accordingly, the most natural choice for the initial state is the thermal state

$$\rho_{\text{th}} = \frac{1}{\mathcal{Z}} e^{-\beta \mathcal{H}}. \quad (2)$$

In our model, the Hamiltonian \mathcal{H} is given by Eq. (1). Here, β and $\mathcal{Z} = \text{tr } e^{-\beta \mathcal{H}}$ are the inverse temperature and the partition function, respectively. Notice that state (2) is a separable state with respect to any bipartition of the system. The physical parameters in Eq. (2) are the number of the qubit N , the Zeeman energy of the i th qubit $h\nu_i$, and the inverse temperature β , which are regarded as the free parameters. Actually, the values of the parameters are restricted by the experiments for a liquid-state NMR quantum computing. For the comparison with Ref. [3], we introduce the parameter $\alpha_i = \beta h\nu_i/2$, which is called a measure of the state's polarization in

the reference. Hereafter, we simply call it polarization. The physical meaning of α_i is quite clear. Let us consider the expectation value of J_z with respect to ρ_{th} : $m_z \equiv \text{tr}(J_z \rho_{\text{th}}) = -\sum_{i=1}^N (\tanh \alpha_i)/2$. We assume the value of N is fixed. The value of $|m_z|$ is large as α_i increases; the system is strongly polarized in the direction of the z axis. Summarizing the above argument, we can say that the initial thermal state (2) is characterized by the number of qubits N and the polarization α_i . Notice that the authors in Ref. [3] assume every α_i is a common value; equation (2) and J_z commute in this case.

Next, we explain the unitary operators for generating entanglement. We will have to investigate all types of the quantum gates which are considered as the generator of entanglement and essential parts in a quantum algorithm. However, this task will be very difficult. In this paper, as in Ref. [3], we concentrate on the following two unitary operators: the controlled-NOT-Hadamard (CH) transformation, $U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I)$, and the CH-fanout transformation, $U_{\text{CF}} = U_{\text{CH}}U_{\text{fan}}$. The fanout gate U_{fan} is defined as follows: $U_{\text{fan}} = |0\rangle_1\langle 0| \otimes I + |1\rangle_1\langle 1| \otimes X$, where $I = \bigotimes_{i=2}^N I_i$, $X = \bigotimes_{i=2}^N X_i$. The above unitary operators are examples in quantum gates, but they include the essential quantum gates for the generation of entanglement: controlled-NOT gates and Hadamard gates. In this case, they generate the entanglement between the first qubit and the remaining qubits. When we consider, for example, the case of $N = 3$ and that the initial state is $|000\rangle = |0\rangle_1 \otimes |0\rangle_2 \otimes |0\rangle_3$, we obtain the following results: $U_{\text{CH}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ and $U_{\text{CF}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$.

In summary, we examine the entanglement of the states

$$\rho_{\text{CH}} = U_{\text{CH}}\rho_{\text{th}}U_{\text{CH}}^\dagger, \quad (3)$$

$$\rho_{\text{CF}} = U_{\text{CF}}\rho_{\text{th}}U_{\text{CF}}^\dagger. \quad (4)$$

We call the above states the Bell-transformed thermal states. The initial state ρ_{th} is separable with any bipartition of the system for the arbitrary values of N and $\{\alpha_i\}_{i=1}^N$.

III. ENTANGLEMENT OF BELL-TRANSFORMED THERMAL STATES WITH CHEMICAL SHIFT

A. Specification of a bipartition

In order to study the entanglement of a system, it is necessary to specify the way to divide it into two parts. We divide the N -qubit system into two subsystems, party A and party B, in the following. First, let us consider a set of binary numbers, $\{k_i\}_{i=1}^N$ ($k_i = 0, 1$). When $k_i = 0$, let the i th qubit be in party A. On the other hand, when $k_i = 1$, it is in party B. We always set $k_1 = 0$; the first qubit is always in party A. For convenience, we introduce an integer $k = \sum_{i=2}^N k_i 2^{i-2}$. Therefore, a partition is specified if an integer k ($\in [1, 2^{N-1}-1]$) is chosen;

we call such a partition the bipartition k . Let us choose, for instance, $k = 4$ in the case of $N = 4$ (i.e., $k_2 = 0$, $k_3 = 0$, and $k_4 = 1$). The elements of party A are the 1st, 2nd, and 3rd qubit, and party B contains only the 4th qubit.

B. PPT criterion

The PPT criterion is the simple and computable way to investigate entanglement. We briefly summarize it. Let us consider a density matrix ρ in a quantum system with finite dimension d . The total system is divided into two subsystems, system A and system B. Introducing an orthonormal basis of the system A, $\{|u_i\rangle_A\}_{i=1}^{d_A}$ and the system B, $\{|v_k\rangle_B\}_{k=1}^{d_B}$, we can expand the density matrix ρ as follows:

$$\rho = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} C(ik|jl) |u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|, \quad (5)$$

where $C(ik|jl)$ is a complex number and $d = d_A d_B$. Next, using Eq. (5), we define the partial transposition of the density matrix with respect to the system B as

$$\rho^{\text{T}_B} = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} C(il|jk) |u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|. \quad (6)$$

Then, we calculate the eigenvalues of ρ^{T_B} and investigate their positivity. If all eigenvalues of Eq. (6) are positive (i.e., $\rho^{\text{T}_B} \geq 0$), it is called a density matrix with PPT. On the other hand, if at least one eigenvalue of it is negative, it is called a density matrix with negative partial transposition (NPT). The most important thing is that there is the following criterion (i.e., PPT criterion):

$$\rho: \text{separable} \Rightarrow \rho: \text{PPT}, \quad (7)$$

or, equivalently

$$\rho: \text{NPT} \Rightarrow \rho: \text{entangled (nonseparable)}. \quad (8)$$

Moreover, the following statement is also known [10, 11]:

$$\rho: \text{distillable} \Rightarrow \rho: \text{NPT}. \quad (9)$$

C. Bell-diagonal states

Before showing our results, we explain the special class of a density matrix, the Bell-diagonal state. It plays a central role in later discussion.

To begin, let us explain the generalized Greenberger-Horne-Zeilinger (GHZ) state [3, 15] in the N -qubit system

$$|\Psi_j^\pm\rangle = \frac{1}{\sqrt{2}} (|0j\rangle \pm |1\bar{j}\rangle) \quad (0 \leq j \leq 2^{N-1}-1), \quad (10)$$

where $j = \sum_{i=2}^N j_i 2^{i-2}$ for the binary number j_i ($= 0, 1$), $|0j\rangle = |0\rangle_1 \otimes \bigotimes_{i=2}^N |j_i\rangle_i$ and $|1\bar{j}\rangle = |1\rangle_1 \otimes \bigotimes_{i=2}^N |1-j_i\rangle_i$. The symbol \bar{j} means a bit-flip of j : $\bar{j} = 2^{N-1} - 1 - j$. We can easily find the generalized GHZ states are the elements of an orthonormal basis of the Hilbert space corresponding to the N -qubit system.

We introduce the following density matrix:

$$\rho_{\text{BD}} = \sum_{j=0}^{2^{N-1}-1} (\omega_j^+ |\Psi_j^+\rangle \langle \Psi_j^+| + \omega_j^- |\Psi_j^-\rangle \langle \Psi_j^-|), \quad (11)$$

where $\omega_j^\pm = \langle \Psi_j^\pm | \rho_{\text{BD}} | \Psi_j^\pm \rangle$ and $\sum_{j=0}^{2^{N-1}-1} (\omega_j^+ + \omega_j^-) = 1$. Equation (11) is a Bell-diagonal state in an N -qubit system. We will show that ρ_{CH} and ρ_{CF} take the form of Eq. (11) in the next subsection.

The reason why we introduce the Bell-diagonal state is that we can easily obtain its partial transposition. We confirm this in the following procedure. First, let us consider a bipartition k . Secondly, we represent $|\Psi_j^\pm\rangle \langle \Psi_j^\pm|$ in the computational basis: $|\Psi_j^\pm\rangle \langle \Psi_j^\pm| = (|0j\rangle \langle 0j| \pm |0\bar{j}\rangle \langle 1\bar{j}| \pm |1\bar{j}\rangle \langle 0j| + |1\bar{j}\rangle \langle 1\bar{j}|)/2$. The diagonal parts of $|\Psi_j^\pm\rangle \langle \Psi_j^\pm|$ are $|0j\rangle \langle 0j|$ and $|1\bar{j}\rangle \langle 1\bar{j}|$ and are invariant under the partial transposition with respect to party B. The off-diagonal ones are $|0j\rangle \langle 1\bar{j}|$ and $|1\bar{j}\rangle \langle 0j|$ because $j \neq \bar{j}$. If the i th qubit is in party B (i.e., $k_i = 1$), the binary number j of the off-diagonal parts is transformed into $j_i + 1 (= j_i + k_i)$ modulo 2 (e.g., $0 + 1 = 1$ and $1 + 1 = 0$) by partial transposition with respect to party B. On the other hand, if the i th qubit is in the party A (i.e., $k_i = 0$), the corresponding j_i is unchanged; $j_i = j_i + k_i$. As a result, we obtain the following expression: $(|\Psi_j^\pm\rangle \langle \Psi_j^\pm|)^{\text{T}_B} = (|\Psi_j^+\rangle \langle \Psi_j^+| + |\Psi_j^-\rangle \langle \Psi_j^-| \pm |\Psi_{j \oplus k}^+\rangle \langle \Psi_{j \oplus k}^+| \mp |\Psi_{j \oplus k}^-\rangle \langle \Psi_{j \oplus k}^-|)/2$, where $j \oplus k = \sum_{i=2}^N l_i 2^{i-2}$ ($l_i \equiv j_i + k_i \pmod{2}$). Accordingly, the Bell-diagonal state partially transposed with respect to party B is given by

$$\rho_{\text{BD}}^{\text{T}_B} = \sum_{j=0}^{2^{N-1}-1} (\mu_j^+ |\Psi_j^+\rangle \langle \Psi_j^+| + \mu_j^- |\Psi_j^-\rangle \langle \Psi_j^-|), \quad (12)$$

where

$$\mu_j^\pm = \frac{\omega_j^+ + \omega_j^-}{2} \pm \frac{\omega_{j \oplus k}^+ - \omega_{j \oplus k}^-}{2}. \quad (13)$$

D. Sufficient conditions for nonseparability

First of all, let us show Eqs. (3) and (4) are just the Bell-diagonal state. Using the standard relations $(H_1 \otimes I)|0j\rangle = (|0j\rangle + |1\bar{j}\rangle)/\sqrt{2}$, $(H_1 \otimes I)|1j\rangle = (|0j\rangle - |1\bar{j}\rangle)/\sqrt{2}$, $U_{\text{fan}}|0j\rangle = |0j\rangle$, and $U_{\text{fan}}|1j\rangle = |1\bar{j}\rangle$, we obtain the following results:

$$\langle \Psi_j^\pm | \rho_{\text{CH}} | \Psi_{j'}^\pm \rangle = \frac{\delta_{jj'}}{\mathcal{Z}} e^{\mp \alpha_1} e^{-\sum_{i=2}^N (-1)^{j_i} \alpha_i}, \quad (14)$$

$$\langle \Psi_j^\pm | \rho_{\text{CF}} | \Psi_{j'}^\pm \rangle = \frac{\delta_{jj'}}{\mathcal{Z}} e^{\mp \alpha_1} e^{\mp \sum_{i=2}^N (-1)^{j_i} \alpha_i}, \quad (15)$$

$$\langle \Psi_j^\pm | \rho_{\text{CH}} | \Psi_{j'}^\mp \rangle = \langle \Psi_j^\pm | \rho_{\text{CF}} | \Psi_{j'}^\mp \rangle = 0, \quad (16)$$

where $0 \leq j, j' \leq 2^{N-1} - 1$. Consequently, both ρ_{CH} and ρ_{CF} are Bell-diagonal states.

Let us define the mean values of the polarization of party A, ξ and party B, η for given j and k as follows:

$$\xi = \frac{1}{N-w} \sum_{i \in A_k} (-1)^{j_i} \alpha_i, \quad \eta = \frac{1}{w} \sum_{i \in B_k} (-1)^{j_i} \alpha_i, \quad (17)$$

where $A_k = \{i \in \mathbb{Z}; k_i = 0, 1 \leq i \leq N\}$, $B_k = \{i \in \mathbb{Z}; k_i = 1, 1 \leq i \leq N\}$. In Eq. (17), we conventionally assign zero to j_1 . The number w is the total number of the elements of party B ($1 \leq w \leq N-1$). In other words, it is the hamming weight of k (i.e., the number of one in $\{k_i\}_{i=1}^N$). Each of ξ and η is a function of j if N , $\{\alpha_i\}_{i=1}^N$, and k are fixed.

Then, we calculate the eigenvalues of $\rho_{\text{CH}}^{\text{T}_B}$ and $\rho_{\text{CF}}^{\text{T}_B}$ with respect to the bipartition k . Now that we know the general expression (13) for the partially transposed Bell-diagonal state, we easily obtain the desired results. For a given bipartition k , the eigenvalue of $\rho_{\text{CH}}^{\text{T}_B}$ is given by

$$\mu_{\text{CH},j}^\pm = \frac{1}{\mathcal{Z}} e^{\alpha_1} \cosh \alpha_1 e^{-(N-w)\xi} n_{\text{CH}}^\pm(\eta), \quad (18)$$

where

$$n_{\text{CH}}^\pm(\eta) = e^{-w\eta} \mp \tanh \alpha_1 e^{w\eta}. \quad (19)$$

Similary, the eigenvalue of $\rho_{\text{CF}}^{\text{T}_B}$ is given by

$$\mu_{\text{CF},j}^\pm = \frac{1}{\mathcal{Z}} n_{\text{CF}}^\pm(\xi, \eta), \quad (20)$$

where

$$n_{\text{CF}}^\pm(\xi, \eta) = e^{\mp(N-w)\xi} \cosh(w\eta) \pm e^{\pm(N-w)\xi} \sinh(w\eta). \quad (21)$$

Hereafter, we assume that α_i s are positive, though generally, their relative signs can be different. For the latter discussion, we evaluate the range of ξ and η for the given $\{\alpha_i\}_{i=1}^N$ and k . We readily obtain the inequalities

$$|\xi| \leq \frac{1}{N-w} \sum_{i \in A_k} \alpha_i \equiv \xi_*, \quad |\eta| \leq \frac{1}{w} \sum_{i \in B_k} \alpha_i \equiv \eta_*. \quad (22)$$

The condition for $\xi = \xi_*$ ($\equiv \xi_{\text{max}}$) is easily found: $j_i = 0$ for any $i \in A_k$. Similarly, the conditions for $\eta = \eta_*$ ($\equiv \eta_{\text{max}}$) and $\eta = -\eta_*$ ($\equiv \eta_{\text{min}}$) are given by $j_i = 0$ and $j_i = 1$ for any $i \in B_k$, respectively. Notice that the value of ξ can't be $-\xi_*$ because $j_1 = 0$; the minimum value of ξ is $-\xi_* + 2\alpha_1/(N-w) \equiv \xi_{\text{min}}$.

Now, we analytically derive the sufficient conditions for the nonseparability of ρ_{CH} and ρ_{CF} . What is needed is that we search for the minimum values of the eigenvalues which can be negative.

First, we examine Eq. (18). We find that the eigenvalue $\mu_{\text{CH},j}^-$ is always positive because all factors of the

right hand side are positive. Then we focus on $\mu_{\text{CH},j}^+$. The positivity is determined by the value of $n_{\text{CH}}^+(\eta)$. Notice that it is a monotonic decreasing function of η , because $\partial n_{\text{CH}}^+(\eta)/\partial \eta < 0$. Therefore, the minimum value of $n_{\text{CH}}^+(\eta)$ is given by $n_{\text{CH}}^+(\eta_{\text{max}}) = n_{\text{CH}}^+(\eta_*) = e^{-w\eta_*} - \tanh \alpha_1 e^{w\eta_*}$. Summarizing the above argument, we can say that ρ_{CH} is NPT with respect to the bipartition k if and only if

$$n_{\text{CH}}^+(\eta_*) < 0 \iff e^{-2w\eta_*} < \tanh \alpha_1. \quad (23)$$

Secondly, let us consider Eq. (20). We concentrate on the behavior of $n_{\text{CF}}^\pm(\xi, \eta)$ because $\mathcal{Z} > 0$. First, we investigate $n_{\text{CF}}^+(\xi, \eta)$. Notice that the value is always positive for $\eta \geq 0$ or $\xi, \eta \leq 0$. Hereafter, we consider the case of $\xi > 0$ and $\eta < 0$. In this case, we find $\partial n_{\text{CF}}^+(\xi, \eta)/\partial \xi < 0$ and $\partial n_{\text{CF}}^+(\xi, \eta)/\partial \eta > 0$. Therefore, the minimum value of $n_{\text{CF}}^+(\xi, \eta)$ is given by $n_{\text{CF}}^+(\xi_{\text{max}}, \eta_{\text{min}}) = n_{\text{CF}}^+(\xi_*, -\eta_*) = e^{-(N-w)\xi_*} \cosh(w\eta_*) - e^{(N-w)\xi_*} \sinh(w\eta_*)$. Next, we consider $n_{\text{CF}}^-(\xi, \eta)$. It should be noted that the following relation is fulfilled: $n_{\text{CF}}^+(\xi, \eta) = n_{\text{CF}}^-(\xi, -\eta)$. Therefore, we readily obtain the information on $n_{\text{CF}}^-(\xi, \eta)$. Through the above arguments, the minimum value of $n_{\text{CF}}^-(\xi, \eta)$ is given by $n_{\text{CF}}^-(\xi_{\text{min}}, \eta_{\text{max}}) = n_{\text{CF}}^-(\xi_{\text{min}}, \eta_*) = e^{-(N-w)\xi_* + 2\alpha_1} \cosh(w\eta_*) - e^{(N-w)\xi_* - 2\alpha_1} \sinh(w\eta_*)$. On the other hand, $n_{\text{CF}}^-(\xi_{\text{min}}, \eta_*)$ is clearly greater than $n_{\text{CF}}^+(\xi_*, -\eta_*)$. Consequently, ρ_{CF} is NPT with respect to the bipartition k if and only if

$$\begin{aligned} n_{\text{CF}}^+(\xi_*, -\eta_*) < 0 \\ \iff \cosh[(N-w)\xi_* - w\eta_*] < \sinh(N\bar{\alpha}), \end{aligned} \quad (24)$$

where $N\bar{\alpha} = \sum_{i=1}^N \alpha_i = (N-w)\xi_* + w\eta_*$.

Let us summarize the sufficient conditions for the non-separability of ρ_{CH} and ρ_{CF} . With respect to the bipartition k , ρ_{CH} is an entangled state if the inequality (23) is fulfilled, and ρ_{CF} is an entangled one if the inequality (24) is fulfilled. The sufficient condition for the non-separability of ρ_{CH} is given by α_1 and the mean value of the polarization of the party B, η_* ; it doesn't depend on α_i ($i \in A_k$) in party A, except for α_1 . On the other hand, the one of ρ_{CF} is determined by ξ_* and η_* ; it depends on the mean values of the polarization for party A and party B.

We have two comments on the above results. As has been mentioned, every α_i is assumed to be positive. Even if that is not the case, the analytical expressions (18) and (20) don't change. However, the least values of $n_{\text{CH}}^\pm(\xi, \eta)$ and $n_{\text{CF}}^\pm(\xi, \eta)$ must be modified. Secondly, if every α_i is a common value, we can readily check that both sufficient conditions (23) and (24) are equivalent to the corresponding results in Ref. [3].

IV. FULL SEPARABILITY AND FULL DISTILLABILITY

Let us consider a N -particle system. A state of this system is called fully separable (or, N -separable) if the corresponding density matrix ρ can be written as a convex combination of direct product states:

$$\rho = \sum_i p_i \bigotimes_{j=1}^N \rho_i^{(j)} \quad \left(\sum_i p_i = 1, p_i \geq 0 \right), \quad (25)$$

where $\rho_i^{(j)}$ is the density matrix on the partial Hilbert space corresponding to the j th particle [15, 17]. One can easily check that a density matrix has PPT with respect to any bipartition of the system if it is fully separable. On the other hand, we call ρ fully distillable if it is distillable with respect to any bipartition (i.e., we can create a maximal entangled pair between qubits in party A and party B by a number of the copies and LOCC), according to Ref. [3]. Through statement (9), we can readily show that a density matrix has NPT with respect to any bipartition, if it is fully distillable.

As in Ref. [3], we examine the full separability and the full distillability of ρ_{CH} and ρ_{CF} . We summarize the necessary condition for the separability of ρ_{CH} and ρ_{CF} . According to Eqs. (23) and (24), the necessary conditions for the separability of ρ_{CH} and ρ_{CF} , respectively, with respect to the bipartition k are given by

$$e^{-2w\eta_*} \geq \tanh \alpha_1, \quad (26)$$

$$\cosh[(N-w)\xi_* - w\eta_*] \geq \sinh(N\bar{\alpha}). \quad (27)$$

Moreover, from Eq. (9), we find that the necessary conditions for the distillability of ρ_{CH} and ρ_{CF} with respect to the bipartition k are given by Eqs. (23) and (24), respectively. Note that the equalities of Eqs. (26) and (27) give the boundaries between the separability and the distillability.

Let us consider the full separability and the full distillability of ρ_{CH} . The necessary condition for the full separability and the full distillability is given by $\min_k (e^{-2w\eta_*}) \geq \tanh \alpha_1$ and $\max_k (e^{-2w\eta_*}) < \tanh \alpha_1$, respectively. In conclusion, we obtain the necessary conditions for the full separability and the full distillability of ρ_{CH} as follows:

$$\rho_{\text{CH}}: \text{fully separable} \Rightarrow e^{-2b_{\text{max}}} \geq \tanh \alpha_1, \quad (28)$$

$$\rho_{\text{CH}}: \text{fully distillable} \Rightarrow e^{-2b_{\text{min}}} < \tanh \alpha_1, \quad (29)$$

where $b_{\text{max}} = \max_k (w\eta_*) = N\bar{\alpha} - \alpha_1$ and $b_{\text{min}} = \min_k (w\eta_*) = \min_{i \neq 1} (\alpha_i)$. The value of $w\eta_*$ takes the maximum value b_{max} when $k = 2^{N-1} - 1$ (i.e., $w = N - 1$). On the other hand, it takes the minimum value b_{min} when k_i corresponding to the minimum value of α_i is 1 and the remainders are 0 (i.e., $w = 1$).

Similarly, we obtain the following results for ρ_{CF} :

$$\rho_{\text{CF}}: \text{fully separable} \Rightarrow \cosh d_{\text{min}} \geq \sinh(N\bar{\alpha}), \quad (30)$$

$$\rho_{\text{CF}}: \text{fully distillable} \Rightarrow \cosh d_{\text{max}} < \sinh(N\bar{\alpha}), \quad (31)$$

where $d_{max} = \max_k |(N-w)\xi_* - w\eta_*|$ and $d_{min} = \min_k |(N-w)\xi_* - w\eta_*|$. The value of $|(N-w)\xi_* - w\eta_*|$ takes the maximum value, d_{max} , when the difference between $(N-w)\xi_*$ and $w\eta_*$ is the largest. If $\alpha_i = \alpha$ for any i , the condition for d_{max} is quite simple. The value of d_{max} is $(N-2)\alpha$, where $k = 2^{N-1} - 1$ (i.e., $w = N-1$) or $k = 1$ (i.e., $w = N-1$). On the other hand, it takes the minimum value, d_{min} when $(N-w)\xi_*$ is the closest value to $w\eta_*$. If every α_i is a common value, the value of d_{min} is 0, where $w = \lfloor N/2 \rfloor$. Here, the symbol $\lfloor x \rfloor$ means the greatest integer that is less than or equal to $x \in \mathbb{R}$.

Our results (28)–(31) are the necessary conditions for the full separability or the full distillability. When all of α_i s are equal, the authors in Ref. [3] showed the sufficient condition for the full distillability, through the statements proved in Ref. [15]. In this case, combining our results (29) and (31) with theirs, we can obtain the following important results:

$$\rho_{CH}: \text{fully distillable} \iff e^{-2\alpha} < \tanh \alpha, \quad (32)$$

$$\rho_{CF}: \text{fully distillable} \iff \tanh \alpha > e^{-2(N-1)\alpha}, \quad (33)$$

(We can find that the necessary condition for the full distillability of ρ_{CF} is $\cosh[(N-2)\alpha] < \sinh(N\alpha)$ from Eq. (31) and this inequality is equal to the corresponding expression in Eq. (33) after a short calculation). Therefore, we obtain the complete physical parameter regions in which ρ_{CH} and ρ_{CF} can be useful for QIP.

V. BOUNDARY BETWEEN SEPARABILITY AND NONSEPARABILITY

The equalities in the inequalities (26) and (27) imply the boundary between the separability and the nonseparability in term of the PPT criterion. We investigate the effect of the chemical shift on such boundaries.

Through the above argument, we easily obtain the following expression of the boundary for ρ_{CH} :

$$e^{-2w\eta_*} = \tanh \alpha_1. \quad (34)$$

Similarly, the boundary for ρ_{CF} is given by

$$\cosh[(N-w)\xi_* - w\eta_*] = \sinh(N\bar{\alpha}). \quad (35)$$

To compare the boundaries with the chemical shift to those without it, we try a toy model for α_i . The polarization α_i divides into a reference value $\alpha (> 0)$ and the deviation $\delta\alpha_i$ from it: $\alpha_i = \alpha + \delta\alpha_i$. Here, we regard $x_i \equiv \delta\alpha_i/\alpha$ as a uniform random variable in $[-\delta, \delta]$ ($0 \leq \delta < 1$). Therefore, in our toy model, the polarization of the i th qubit is given by $\alpha_i = \alpha(1 + x_i)$. Furthermore, the value of α is regarded as the mean value of polarization.

Let us explain how to calculate the boundaries. In the first, we choose the value of δ ; actually, $\delta = 0.1, 0.01$, and 0. Then, a sequence of random numbers in $[-\delta, \delta]$ is

generated by the Mersenne Twister [18]. Next, we specify a bipartition. For the sake of simplicity, we assume the first $N-w$ qubits are in the party A and the latter w qubits are in party B. Finally, we numerically calculate the value of α satisfying with Eqs. (34) or (35) for a given N by the bisection method.

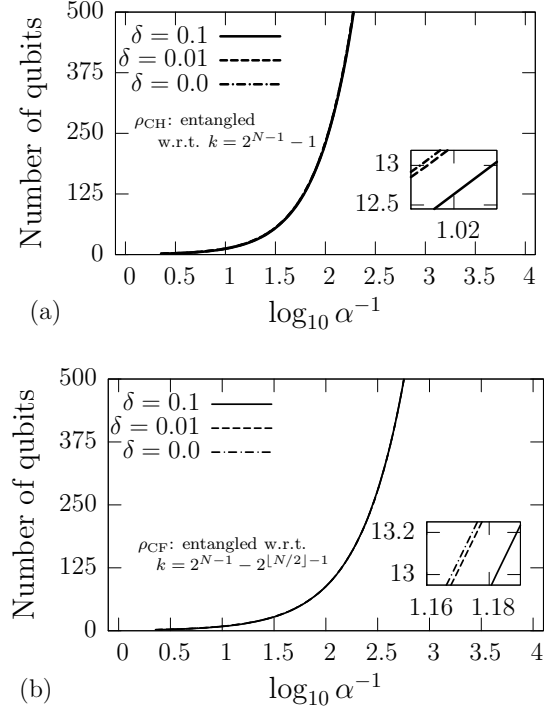


FIG. 1: Boundary between the separability and the nonseparability in term of the PPT criterion. The solid line is for $\delta = 0.1$, the broken line is for $\delta = 0.01$, and the broken dotted line is for $\delta = 0$; actually, the difference between these is very small (see the insets). (a) The CH transformation ($k = 2^{N-1} - 1$). (b) The CH-fanout transformation ($k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$).

In Figs. 1(a) and (b), we show the boundaries on (α, N) plan for a specific sequence of x_i . The horizontal axis is the common logarithm of the inverse of α . The larger value of $\log_{10} \alpha^{-1}$ corresponds to the case of the higher temperature. The longitudinal axis is the number of qubits. The solid line, the broken line, and the broken dotted line correspond to the boundaries for $\delta = 0.1$, $\delta = 0.01$, and $\delta = 0$, respectively. We show the results for ρ_{CH} with respect to a bipartition $k = 2^{N-1} - 1$ (i.e., $w = N-1$) in Fig. 1(a), and the case of ρ_{CF} with respect to a bipartition $k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$ (i.e., $w = \lfloor N/2 \rfloor$) in Fig. 1(b). The left sides of those lines are the parameter regions where ρ_{CH} and ρ_{CF} are nonseparable with respect to the corresponding bipartition. We find that the clear distinction among the different values of δ is invisible in both Figs. 1 (a) and (b); for example, denoting the value of α on the boundary as $\alpha_b(\delta)$ for a given δ , we can find that $|\log_{10} [\alpha_b(0)/\alpha_b(\delta)]| \leq 10^{-2}$ for $\delta = 0.1$ and 0.01 , as N is large. In addition, we can find a similar behavior even if we change the sequence of random variables

and the kind of bipartitions. Consequently, the effect of the chemical shift on the boundary between the separability and the nonseparability is negligible in our model for $\{\alpha_i\}_{i=1}^N$. This result implies that one have only to examine the number of qubits N and the mean value of polarization α for the determination of the entanglement of the Bell-transformed thermal states (3) and (4).

Let us consider the reason why the effect of the chemical shift is negligible. The boundaries for both ρ_{CH} and ρ_{CF} between the separability and the nonseparability are given by Eqs. (34) and (35), respectively. Those equations are mainly determined by the mean values of the polarization of party A, ξ_* and party B, η_* . Therefore, the deviation from the mean value of α_i s is not important for the determination of the boundaries.

When the chemical shift occurs, the thermal state ρ_{th} and J_z do not commute; the symmetry of the system is lower than the one without it. According to the above arguments, the effect of the chemical shift on the boundary between the separability and the nonseparability isn't found. Our analysis has not revealed the relation between the symmetry and the generation of entanglement by quantum dynamics. However, the model for α_i is quite simple; the distribution of α_i is uniform and random. We have also assumed that α_i s are positive. Therefore, it is necessary to investigate a more general and realistic model for α_i to clarify this relation.

VI. SUMMARY

We have analytically derived the physical parameter region where the Bell-transformed thermal states are entangled in the presence of the chemical shift, by the use of the PPT criterion with respect to any bipartition. Two kinds of Bell-transformations, the CH transformation U_{CH} and the CH-fanout transformation U_{CF} , have been examined, as in Ref. [3]. With respect to the bipartition k , ρ_{CH} is an entangled state if the inequality (23) is fulfilled, and ρ_{CF} is an entangled one if the inequality (24) is fulfilled. If the every α_i is a common value, our results are equal to the corresponding ones in Ref. [3]. There exists an obvious differences between Eqs. (23) and (24) with respect to their dependence on α_i . The sufficient condition for the nonseparability of ρ_{CH} is given by α_1 and the mean value of the polarization of the party B, η_* ; it doesn't depend on α_i ($i \in A_k$) in party A, except for α_1 . On the other hand, the one of ρ_{CF} is determined by ξ_* and η_* ; it depends on the mean values of the polarization for party A and party B.

Next, we have derived the necessary conditions for the full separability and the full distillability through the above analytical results. On the other hand, the authors in Ref. [3] obtained the sufficient conditions when all of α_i s are equal. We have obtained the necessary and sufficient conditions for the full distillability of ρ_{CH} and ρ_{CF} in this case, combining our results with theirs. Accordingly, we can completely characterize the physical param-

eter regions in which those unitary transformed thermal states can be useful for QIP, if there is no chemical shift. When the chemical shift exists, we will have to examine the sufficiency of our results.

Finally, we have investigated the effect of the chemical shift on the boundary between the separability and the nonseparability determined by the PPT criterion. We have shown such an effect on the boundaries should be negligible. Actually, one have only to know the number of qubits N and the mean value of polarization α for the evaluation of the entanglement of the Bell-transformed thermal states (3) and (4). This result is quite natural, because the boundaries for both ρ_{CH} and ρ_{CF} between the separability and the nonseparability dominantly depend on the mean values of the polarization of party A, ξ_* and party B, η_* . The thermal state is a more elementary state than effective pure states in liquid-state NMR. We have attempted to reveal the connection between the symmetry of the thermal state and the property of quantum gates (i.e., quantum dynamics) in terms of entanglement. Our analyses have not clarified this point. We will research a more general and realistic model for α_i .

It is also important to examine the difference between ρ_{CH} and ρ_{CF} (i.e., U_{CH} and U_{CF}) in terms of the entanglement generation. The authors in Ref. [3] concluded that U_{CF} is a more effective Bell-transformation than U_{CH} because the parameter region in which ρ_{CF} is fully distillable is wider than the corresponding one of ρ_{CH} . In this paper, we have obtained the analytical expressions of the eigenvalues of ρ_{CH}^{TB} and ρ_{CF}^{TB} . Therefore, the results allow us to characterize U_{CH} and U_{CF} in more detail; for instance, we can evaluate the negativity, which is an entanglement measure [19, 20]. We will show the results in the near future.

Research on entanglement in liquid-state NMR involves various aspects of quantum information theory, for example, the role of mixed states in quantum computing and the classification of entanglement. One should note that the achievable range of the physical parameters N and α_i s is limited in a current liquid-state NMR experiment. Actually, it may be difficult to compare the theoretical results with the experiments. However, several experimental developments have been reported in liquid-state NMR, for example, the highly polarized initial states [21] and the number of qubits greater than ten [22, 23]. Furthermore, research on a solid-state NMR quantum computer [24], which can relax the limitation of liquid-state NMR, has been developed steadily. Consequently, we expect that theoretical research on the entanglement in liquid-state NMR could be connected with these experiments in future.

Acknowledgments

The authors acknowledge H. Nakazato for valuable discussions. One of the authors (Y. O.) greatly acknowledges the discussion with T. Y. Petrosky, N. Hatano,

and M. Machida. One of the authors (S. M.) thanks Y. Tanaka. This research is partially supported by a Grant-in-Aid for Priority Area B (No. 763), MEXT, and one for the 21st-Century COE Program (Physics of Self-Organization Systems) at Waseda University from MEXT, and by a Waseda University Grant for Special Research Projects (No. 2004B-872).

APPENDIX A: NOTES ON DÜR-CIRAC CLASSIFICATION

The Dür-Cirac classification [15] is a very effective way to evaluate the separability or the distillability of density matrices, of either pure or mixed states, in a multiqubit system, and it is widely used [3, 17, 25]. However, we have to take care to use it; we don't always obtain information on their entanglement from the method proposed in Ref. [15]. In the appendix, we show several examples in which the method doesn't work. Unfortunately, we don't know what kind of density matrices have the problem. Nevertheless, in the end of the appendix, we propose the prescription to solve this problem in specific examples.

First of all, we summarize the strategy of the Dür-Cirac classification. In order to evaluate the entanglement of a quantum state by the PPT criterion, one must examine the positivity of the partial transposed density matrices. In general, such tasks will be difficult as the number of qubits becomes large and many choices of bipartitions exist. On the other hand, if one uses the Dür-Cirac classification, it is only necessary to calculate some specific matrix elements of the state concerned. The main idea is that, using a sequence of local operations, one can transform an arbitrary density matrix ρ in a N -qubit system into the following state whose property of entanglement is easily examined:

$$\rho_N = \lambda_0^+ |\Psi_0^+\rangle\langle\Psi_0^+| + \lambda_0^- |\Psi_0^-\rangle\langle\Psi_0^-| + \sum_{j=1}^{2^{N-1}-1} \lambda_j (|\Psi_j^+\rangle\langle\Psi_j^+| + |\Psi_j^-\rangle\langle\Psi_j^-|). \quad (\text{A1})$$

The original density matrix ρ is related to ρ_N by the following expressions: $\lambda_0^\pm = \langle\Psi_0^\pm|\rho|\Psi_0^\pm\rangle$ and $2\lambda_j = \langle\Psi_j^+|\rho|\Psi_j^+\rangle + \langle\Psi_j^-|\rho|\Psi_j^-\rangle$. The property of ρ_N is characterized as follows:

$$\rho_N: \text{PPT with a bipartition } k \iff \Delta \leq 2\lambda_k, \quad (\text{A2})$$

or

$$\rho_N: \text{NPT with a bipartition } k \iff \Delta > 2\lambda_k, \quad (\text{A3})$$

where $\Delta = |\lambda_0^+ - \lambda_0^-|$. The most important key idea is that the entanglement does not increase through local operations. Accordingly, if ρ_N is a nonseparable state with a bipartition, ρ is also such a state. It should be noticed that we obtain information on the entanglement of ρ only if ρ_N is a nonseparable state.

Now, we show three examples. The first one is the case in which the Dür-Cirac classification works well. The remaining two are not such cases. Hereafter, we concentrate on a two-qubit system. Therefore, the value of k in Eqs. (A2) and (A3) is always 1. In the first, let us consider the following state:

$$\rho_{iso} = (1-f)\frac{1}{4}(I_1 \otimes I_2) + f|\Psi_0^+\rangle\langle\Psi_0^+|, \quad (\text{A4})$$

where $-1/3 \leq f \leq 1$. The above density matrix is called an isotropic state [11]. Directly using the PPT criterion [13, 14], we readily find ρ_{iso} is an entangled state if $f > 1/3$. On the other hand, we apply the Dür-Cirac method to ρ_{iso} . We obtain the following results: $\langle\Psi_0^+|\rho_{iso}|\Psi_0^+\rangle = (1+3f)/4$, $\langle\Psi_0^-|\rho_{iso}|\Psi_0^-\rangle = (1-f)/4$, and $\langle\Psi_1^+|\rho_{iso}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho_{iso}|\Psi_1^-\rangle = (1-f)/2$. Accordingly, using Eq. (A3), we also find ρ_{iso} is an entangled one if $f > 1/3$.

Next, we consider a slight different state from ρ_{iso}

$$\rho'_{iso} = (1-f)\frac{1}{4}(I_1 \otimes I_2) + f|\Psi_1^+\rangle\langle\Psi_1^+|, \quad (\text{A5})$$

where $-1/3 \leq f \leq 1$. Notice that the condition for the nonseparability of ρ'_{iso} is the same one as ρ_{iso} ; ρ'_{iso} is an entangled state if $f > 1/3$. This result is quite natural, because the state ρ_{iso} is transformed into ρ'_{iso} by a local unitary operator; $\rho'_{iso} = (I_1 \otimes X_2)\rho_{iso}(I_1 \otimes X_2)^\dagger$. On the other hand, we obtain the eigenvalues in the form of Eq. (A1) as follows: $\langle\Psi_0^+|\rho'_{iso}|\Psi_0^+\rangle = (1-f)/4$, $\langle\Psi_0^-|\rho'_{iso}|\Psi_0^-\rangle = (1-f)/4$, and $\langle\Psi_1^+|\rho'_{iso}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho'_{iso}|\Psi_1^-\rangle = (1+f)/2$. Therefore, the value of Δ is less than $2\lambda_1$ for the arbitrary value of f and the condition (A2) is satisfied. This might imply that ρ'_{iso} is always separable. However, ρ'_{iso} is local unitary equivalent to the entangled state ρ_{iso} ($f > 1/3$). In conclusion, we can't obtain information on the entanglement of ρ'_{iso} by the method in Ref. [15], because the entangled state ρ'_{iso} is transformed into a separable state by LOCC.

The third example is related to the task in this paper. We consider the case of $N = 2$ and $\alpha_1 = \alpha_2 = \alpha$ in Eq. (3). We have known the condition for the nonseparability of ρ_{CH} ; ρ_{CH} is an entangled state if $e^{-2\alpha} > \tanh \alpha$. However, the value of Δ is less than $2\lambda_1$ for any α because $\langle\Psi_0^+|\rho_{CH}|\Psi_0^+\rangle = e^{-2\alpha}/\mathcal{Z}$, $\langle\Psi_0^-|\rho_{CH}|\Psi_0^-\rangle = 1/\mathcal{Z}$ and $\langle\Psi_1^+|\rho_{CH}|\Psi_1^+\rangle + \langle\Psi_1^-|\rho_{CH}|\Psi_1^-\rangle = (1+e^{2\alpha})/\mathcal{Z}$. Accordingly, we can't also obtain information on the entanglement of ρ_{CH} by the method in Ref. [15].

The authors in Ref. [3] pointed out that the local operations can decrease the entanglement of the state concerned and an alternative method is necessary. In particular, they discussed a more effective procedure for evaluating entanglement than the local operations in the Dür-Cirac classification in terms of the mathematical theory of majorization. Finally, we comment on a loophole in the Dür-Cirac classification from another point view: We attempt to construct a prescription to solve the problem. As has been mentioned, the isotropic state

ρ_{iso} is transformed into ρ'_{iso} by the local unitary operator $I_1 \otimes X_2$. The method in Ref. [15] works for the former but not for the latter. This suggests that, by suitable local unitary operators, the state for which the Dür–Cirac classification doesn’t work, could be transformed into a proper one to which their method is applicable. Let us consider the above third example. When we use the local unitary operator $I_1 \otimes X_2$, the state concerned is transformed into $\rho'_{CH} = (I_1 \otimes X_2)\rho_{CH}(I_1 \otimes X_2)^\dagger$, where $\langle \Psi_0^+ | \rho'_{CH} | \Psi_0^+ \rangle = 1/\mathcal{Z}$, $\langle \Psi_0^- | \rho'_{CH} | \Psi_0^- \rangle = e^{2\alpha}/\mathcal{Z}$, and $\langle \Psi_1^+ | \rho'_{CH} | \Psi_1^+ \rangle + \langle \Psi_1^- | \rho'_{CH} | \Psi_1^- \rangle = (e^{-2\alpha} + 1)/\mathcal{Z}$. Calculating Δ and $2\lambda_1$, we can obtain the non-trivial expression for ρ'_{CH} ; for example, ρ'_{CH} is NPT if and only if $\sinh(2\alpha) > 1$. If ρ'_{CH} is entangled, the corresponding state ρ_{CH} is also considered to be entangled. Therefore, we obtain the sufficient condition of the nonseparability for ρ_{CH} , by the use of the Dür–Cirac classification; such a condition is just $\sinh(2\alpha) > 1$. This condition is equal to the one which is derived by the use of Eq. (23). It is necessary to examine whether such a prescription is generalized or not.

lating Δ and $2\lambda_1$, we can obtain the non-trivial expression for ρ'_{CH} ; for example, ρ'_{CH} is NPT if and only if $\sinh(2\alpha) > 1$. If ρ'_{CH} is entangled, the corresponding state ρ_{CH} is also considered to be entangled. Therefore, we obtain the sufficient condition of the nonseparability for ρ_{CH} , by the use of the Dür–Cirac classification; such a condition is just $\sinh(2\alpha) > 1$. This condition is equal to the one which is derived by the use of Eq. (23). It is necessary to examine whether such a prescription is generalized or not.

-
- [1] *The Physics of Quantum Information: Quantum Cryptography, Quantum Teleportation, Quantum Computation*, edited by D. Bouwmeester, A. Ekert, and A. Zeilinger (Springer, Berlin, 2000).
 - [2] Y. Shimoni, D. Shapira, and O. Biham, Phys. Rev. A **69**, 062303 (2004); **72**, 062308 (2005).
 - [3] T. M. Yu, K. R. Brown, and I. L. Chuang, Phys. Rev. A **71**, 032341 (2005).
 - [4] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).
 - [5] E. Knill, I. Chuang, and R. Laflamme, Phys. Rev. A **57**, 3348 (1998).
 - [6] I. L. Chuang, N. Gershenfeld., M. G. Kubinec, and D. W. Leung, Proc. R. Soc. Lond. A **454**, 447 (1998).
 - [7] A. Galindo and M. A. Martín-Delgado, Rev. Mod. Phys. **74**, 347 (2002).
 - [8] S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu, and R. Schack, Phys. Rev. Lett. **83**, 1054 (1999).
 - [9] C. H. Bennett, G. Brassard, S. Popescu, B. Schumacher, J. A. Smolin, and W. K. Wootters, Phys. Rev. Lett. **76**, 722 (1995).
 - [10] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Rev. Lett. **80**, 5239 (1998).
 - [11] G. Alber, T. Beth, M. Horodecki, P. Horodecki, R. Horodecki, M. Rötteler, H. Weinfurter, R. Werner, and A. Zeilinger, *Quantum Information: An Introduction to Basic Theoretical Concepts and Experiments* (Springer, Berlin, 2001), Chap.5.
 - [12] L. M. K. Vandersypen and I. L. Chuang, Rev. Mod. Phys. **76**, 1037 (2004).
 - [13] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
 - [14] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223**, 1 (1996); P. Horodecki, *ibid.* **232**, 333 (1997).
 - [15] W. Dür and J. I. Cirac, Phys. Rev. A **61**, 042314 (2000).
 - [16] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, Phys. Rev. Lett. **78**, 2275 (1997).
 - [17] K. Nagata, Phys. Rev. A **66**, 064101 (2002).
 - [18] M. Matsumoto and T. Nishimura, ACM Trans. Model. Comput. Simul. **8**, 3 (1998).
 - [19] K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A **58**, 883 (1998); K. Zyczkowski, Phys. Rev. A **60**, 3496 (1999).
 - [20] G. Vidal and R. F. Werner, Phys. Rev. A **65**, 032314 (2002).
 - [21] M. S. Anwar, D. Blazina, H. A. Carteret, S. B. Duckett, T. K. Halstead, J. A. Jones, C. M. Kozak, and R. J. K. Taylor, Phys. Rev. Lett. **93**, 040501 (2004); M. S. Anwar, J. A. Jones, D. Blazina, S. B. Duckett, and H. A. Carteret, Phys. Rev. A **70**, 032324 (2004).
 - [22] J.-S. Lee and A. K. Khitrin, J. Chem. Phys. **122**, 041101 (2005).
 - [23] C. Negrevergne, T. Mahesh, C. A. Ryan, M. Ditty, F. Cyr-Racine, W. Power, N. Boulant, T. Havel, D. Cory, and R. Laflamme, Phys. Rev. Lett. **96**, 170501 (2006).
 - [24] J. Baugh, O. Moussa, C. A. Ryan, R. Laflamme, C. Ramanathan, T. F. Havel, and D. G. Cory, Phys. Rev. A **73**, 022305 (2006).
 - [25] S. Bandyopadhyay and D. A. Lidar, Phys. Rev. A **72**, 042339 (2005).